

a<sup>2</sup>  
66%, each cell is assigned to a data group as shown in the middle set of three columns. Here it is clear that the order of compounds in this table is systematic (111, 112, etc.), to illustrate that the complete set is present. The third set of three columns shows color coding, with the darkest being least active and the lightest being most active.

Please delete the entire paragraph starting at page 47, line 5 and replace it with the following new paragraph:

a<sup>3</sup>  
Then the data set was processed by the system to yield dose-responsiveness scores, and the results sorted by this score, giving **FIGURE 16G**, the complete set in order of decreasing dose-responsiveness. **FIGURE 16G** also shows the intermediate step-scoring and unscaled score points, to aid in following and understanding the algorithm. These points are not displayed by the system itself.

Please delete the entire paragraph starting at page 47, line 16 and replace it with the following new paragraph:

a<sup>4</sup>  
The data value groups' ordinal index numbers are used as single-point activity measures instead of the original data numbers. Extra weight is given to activity shown at lower concentrations by the simple algorithm of weighting each data column by its serial position, again ignoring the actual concentration values. The scores are then scaled to the range 0 to 100. The results of this scoring on the same complete set are shown in **FIGURE 16H** which has been re-sorted by decreasing overall activity.

Please delete the entire paragraph starting at page 48, line 2 and replace it with the following new paragraph:

a<sup>5</sup>  
Comparison of **FIGURES 16G & 16H** shows clearly that the compound ordering by dose-responsiveness is quite different from the ordering by overall activity. The user (a chemist) could now color-code the new score columns and use them as independent factors in a larger scoring. However, chemists also want a *single* index of compound quality derived from the dose-dependent data. Moreover, a composite index would further help to alleviate the effects of noise on data interpretation, by incorporating more information into the ordering process. This is an "information-based smoothing" of the data. Therefore, a procedure to calculate a third, "smart composite" score from the other two scores was devised.

Please delete the entire paragraph starting at page 49, line 8 and replace it with the following new paragraph:

a6  
The value of the coefficient  $k=0.06$ , for which the activity bias starts to become substantial around an activity score of eighty (80), was chosen for implementation in a preferred embodiment of this invention, according to empirical results. **FIGURE 16I** shows the variation for a few values of  $k$ . **FIGURE 16J** shows all three scores for the example complete set, now sorted by decreasing composite score.

Please delete the entire paragraph starting at page 52, line 24 and replace it with the following new paragraph:

a7  
The result is that the markers are sorted into the list according to their potencies, and the potencies of the other compounds can be estimated by interpolating between the markers, using the composite dose-response scores. To illustrate, a typical section of a sorted list is shown below in **FIGURE 16M**, using four colors.

Please delete the entire paragraph starting at page 53, line 17 and replace it with the following new paragraph:

a8  
**FIGURES 16N** and **16P** show that the estimates are clearly quite good within the range of the testing concentrations (pK 5 to 7), but the quality of estimation deteriorates quickly beyond those limits, and algorithm does not reliably distinguish among compounds whose potencies are more than a half log unit beyond the testing range. Therefore, it was decided that presently preferred embodiments would not report any estimated values that fell outside the range of concentrations used in the testing data columns. Thus, in the example in **FIGURE 16M**, the lowest testing concentration was  $10^{-7}$  M (= 0.1  $\mu$ M). For the first compound in **FIGURE 16M**, the system has estimated a potency with  $pIC_{50} > 7$ , but it conservatively only reports "<0.1  $\mu$ M."

Please delete the entire paragraph starting at page 54, line 4 and replace it with the following new paragraph:

a9  
**TABLE 2** summarizes the statistics of the estimations within the testing limits. **TABLE 2** shows that the method successfully estimates the potencies within about a factor of two, even with high noise levels.

Please delete the table heading at page 54, line 7 and replace it with the following new table heading:

a10  
Table 2. Statistics of Estimation Validations

IN THE DRAWINGS:

Please replace the drawings with the corresponding new color drawings provided with the “Petition Under 37 CFR 1.84(a)(2) Regarding Color Drawings” and included herewith, and including the changes to Figures 16F, 16G, 16H, 16J and 16M as described below.

The changes to Figures 16F, 16G, 16H, 16J and 16M are described as follows:

In Figure 16F, the reference to “Table 2” has been deleted from the legend appearing on the drawing sheet.

In Figure 16G, the reference to “Table 3” has been deleted from the legend appearing on the drawing sheet.

In Figure 16H, the reference to “Table 4” has been deleted from the legend appearing on the drawing sheet.

In Figure 16J, the reference to “Table 5” has been deleted from the legend appearing on the drawing sheet.

In Figure 16M, the reference to “Table 6” has been deleted from the legend appearing on the drawing sheet.